Anti-ferroelectric to Paraelectric Phase Transition in Lead Zirconate Thin Films	X16C

D. Fanning, I. Robinson, D. Payne, T. Tani (U. of Illinois, Urbana-Champaign)

We have studied the anti-ferroelectric to paraelectric phase transition in lead zirconate ($PbZrO_3$) thin films as a function of applied electric field and temperature. The films were prepared by sol gel methods and deposited onto $Pt/Ti/SiO_2/Si$ substrates by spin casting. By varying the texture of the substrate and the amount of Ti, films with both (111) and (100) preferred orientation were grown. These textured films are not completely crystalline and have a random orientation with respect to an axis perpendicular to the film. As a result, the crystallographic peaks lie in rings around the axis of the surface normal, and the diffraction pattern has 'fiber texture.' At room temperature, lead zirconate has the polar space group Pbam. Adjacent unit cells have lead atoms displaced in opposite directions along the pseudocubic [110] directions (Figure 1), making it anti-ferroelectric and creating a superstructure at the (h+1/4, k+1/4, l) positions.

We found the (100) films to be preferentially oriented with the c direction perpendicular to the thin films. By comparing scattering at normal incidence to grazing incidence, we found lattice spacings of 4.173 and 4.130 $\AA$ for the (200) and (002) peaks, respectively. Since the Pt substrate has a lattice constant that is about 5% smaller than PZ, it is surprising that the shorter c-axis would align perpendicular to the film. Another result of the c-axis preference was that superstructure reflections with (h+1/4, k+1/4, L) were quite strong, while reflections with non integer L were weak or non-existent. The superstructure peaks' intensity gradually diminishes with increasing temperature (Figure 2). The dependence of the tetragonal splitting had a similar behavior, and both disappeared at about 220 C in the (111) oriented films and 230 °C in the (100) films. This is in contrast to the bulk behavior where the phase transition is noticeably sharper and occurs at 230 °C.

H Fujishita, J. Phys. Soc. Japan, 53 [1], p. 226, 1984.

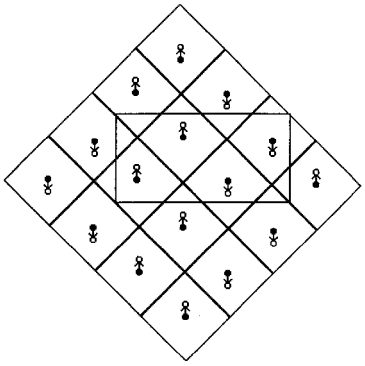

Figure 1.

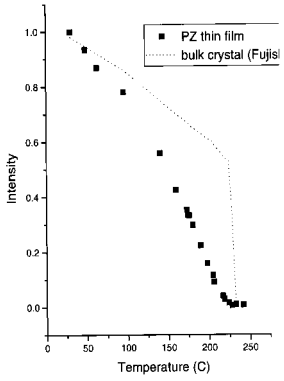

Figure 2.